

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.58e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 4.41e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Fenuron</div> <div>Measured: 2.45e-02</div> <div>Predicted: 2.70e-01</div>	<div>Image not found</div> <div>Phenazone</div> <div>Measured: 2.73e-01</div> <div>Predicted: 1.63</div>	<div>Image not found</div> <div>Dimetan</div> <div>Measured: 1.42e-01</div> <div>Predicted: 9.25e-02</div>
<div>Image not found</div> <div>Furilazole</div> <div>Measured: 7.08e-04</div> <div>Predicted: 7.48e-02</div>		